

Rigidity percolation on aperiodic lattices

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Abstract

We studied the rigidity percolation (RP) model for aperiodic (quasi-crystal) lattices. The RP thresholds (for bond dilution) were obtained for several aperiodic lattices via computer simulation using the “pebble game” algorithm. It was found that the (two rhombi) Penrose lattice is always floppy in view of the RP model. The same was found for the Ammann’s octagonal tiling and the Socolar’s dodecagonal tiling. In order to impose the percolation transition we used so c. “ferro” modification of these aperiodic tilings. We studied as well the “pinwheel” tiling which has “infinitely-fold” orientational symmetry. The obtained estimates for the modified Penrose, Ammann and Socolar lattices are respectively: $p_{cP} = 0.836 \pm 0.002$, $p_{cA} = 0.769 \pm 0.002$, $p_{cS} = 0.938 \pm 0.001$. The bond RP threshold of the pinwheel tiling was estimated to $p_c = 0.69 \pm 0.01$. It was found that these results are very close to the Maxwell (the mean-field like) approximation for them.

Modeling rigidity is a paradigmatic case of physical science as it is classically conceived: the consideration of an elementary mechanical model is used to bring some light in an altogether different realm, for instance the behavior of matter at the atomic scale. In this way the questions why a construction such as the Eiffel Tower is stable or why glasses do not flow[1] are linked together.

In a pioneering work[2] Maxwell sought to know when a mechanical construction of rigid bars and pin joints becomes stable. The answer was: when the number of independent constraints reaches the number of degrees of freedom. But there is a next task, which appeared much more difficult: how one can determine in a very large structure which constraints are independent and which are redundant.

Rigidity is an intuitively clear concept, even though its analysis soon reveals unusual aspects. A triangular frame formed from three bars connected by pin joints is a rigid body, while a square is easily deformed. Regardless of the number

of elementary cells a construction of adjacent triangles is also rigid while made out of squares it is still floppy. But in the latter case the lack of rigidity may be thought as an effect of the finite size: if on a square lattice a periodic (helical) boundary conditions are imposed it would be a rigid construction[3] (see also [4, 5]).

The next step in the analysis lies in the procedure of “network dilution”. If randomly chosen bars are removed from the inside of a sufficiently large rigid structure at some moment it loses this integral property. Obviously it can be carried out in the reverse direction: starting with an unstable construction, bonds are added until it becomes rigid. (One may note here that if it is carried out in an orderly fashion it allows to transform a generic square lattice into a triangular one — or vice versa).

A more general approach considers an arbitrary collection of sites in space – in the plane for instance – which are joined to their nearest neighbors, and to relate the change in behavior with the numbers of possible bonds allowed, i.e. with the coordination number. Indeed the bars and joints picture is a special case of the central-force percolation(CFP) model. In CFP one can change the angles between bonds without cost of energy and any motion which include change of bond lengths would change the energy of the system. So one can differentiate the CFP and bars and joints model (in this paper referred as rigidity percolation). In the later case any changes in the bond lengths are not allowed and the bond angles’ changes are still “zero energy” motions.

So the bars and joints picture could locate the place of the rigid-to-floppy transition but could not give direct information (e.g.) about the the elastic modulus critical behavior. But this model picture has the huge computational advantage to make possible avoiding the forces equilibrium calculations which usually scales with system size(L) at criticality as L^{d+2} and faster (d is the spatial dimension). This advantage was not utilized for a long time since the numerical simulations of this model remained the same as for general central-force percolation — via forces equilibrium calculations.

A recent work by Thorpe & Jacobs [6] proposed an efficient way for overcoming the computational difficulties which arise in rigidity percolation models. Instead of “perfect” lattices – lattices which bond lengths and bond angles are taken from a countable set – their topological equivalents were used: for such “generic” lattices, the connectivity is preserved but each bond and bond angle are taken from continuous distribution. Moreover it is argued that the “perfect” lattices are “atypical” and more natural are their generic counterparts. Thorpe & Jacobs [6, 7] also turned the attention to an efficient combinatorial algorithm[8] for constraints counting called the “pebble game” algorithm (see also [9, 10]. All that made possible estimating the central-force percolation thresholds without solving huge and badly conditioned sets of linear equations.

In this work we present a computer simulation study of the rigidity percolation in aperiodical (quasicrystalline) twodimensional structures. We study the bond-dilution case of percolation on four aperiodic lattices. Three of them

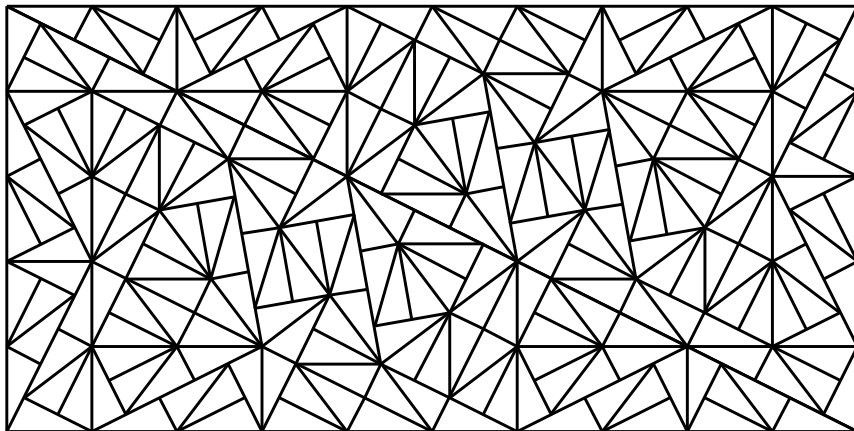


Figure 1: The pinwheel tiling

are modification of aperiodic lattices with "forbidden" orientational symmetry: the two rhombi Penrose tiling (with five-fold symmetry), an octagonal tiling (known as the Ammann's A4 tiling[11]) which is constructed by a square and a rhombus, and a dodecagonal tiling proposed by Socolar[12] constructed by a square, hexagon and a rhombus.

The interest to such tilings came mainly after discovering of the quasicrystals in 1984 [13]. After the first observation of icosahedral quasicrystals, soon after new metal alloys with one periodic axis and 5(10)- 8- and 12-fold orientational symmetry (in the perpendicular plane) were discovered. These four symmetries are likely the only "non-crystallographic" (rotational) symmetries which could be found in nature.

We modified the mentioned lattices by adding bond through these diagonals of the tiles, which are shorter than the tile edge (See Fig.2; and in [14]: Fig. 1c and 1d), the reason for that will be described below. The fourth aperiodic lattice we choose to study was the so c. "pinwheel" tiling[15, 16]: an aperiodic and deterministic tiling which edges are uniformly distributed in all directions (Fig.1) — in this sense — a tiling with "infinitely-fold" orientational order.

Indeed the orientational symmetry could not have direct relation with the rigidity thresholds, since the "pebble game" algorithm which we use does not take in account the bond lengths and orientations. Some indirect relation could be searched in the way the coordination of neighboring sites is correlated. In this study we make comparison only with the mean coordination number. The lattices we study here have coordination numbers between 6 and 4 i.e. they can be ranged somewhere between the paradigmatic cases of triangular and square lattices.

A square lattice according to Maxwell's law would be rigid only if all bonds

are present ($p = 1$) and of course there could not be any redundant bonds in it. The (two rhombi) Penrose lattice, the primer for deterministic aperiodic structure, has also a coordination number $z = 4$ and failed to produce any clue of becoming rigid.

So in order to see a rigidity transition one have to modify the lattice in order to increase its mean coordination number. The most natural modification is to put bonds between the lattice sites if the distance between them is less than the tile edge length. It was coined a name for this: ferromagnetic modification, or, ferro variant of an aperiodic tiling.

The 'ferro variant' of the Penrose tiling has $z = 4.76..$ and one could expect that a rigidity percolation threshold should exist.

The non-modified variants of the octagonal and dodecagonal lattices have mean coordination numbers equal to 4 and 3.63.. respectively [14], so they have to be modified in an analogous way. The ferro variants of these lattices includes new bonds which are the short diagonals of the rhombuses in them. As seen from the table the mean coordination z is 5.17.. and 4.27.. respectively.

The pinwheel tiling consists of identical triangles with sides in the ratio $1 : 2 : \sqrt{5}$ appearing in infinitely many orientations. Inspection of the figure 1 shows that in about one fifth of the cases two of the shortest sides of adjacent triangles are co-linear (forming the side with length 2 units in another triangle) delimiting thus a perimeter with 4 points. So this is a vortex-to-edge tiling. (See the M. Senechal's book in [15])

The question here is how to deal with the vortices which lie on a bond of another triangle. We choose to think that the outer points of the pairs of such co-linear short bonds are also connected. Thus they appear graphically as degenerated triangles of zero area but in this type of study what matters is the topology (connectivity) and not the geometry, (which is emphasized in the concept of generic network). The inclusion of these additional bonds has fixed the theoretical coordination number to 6. In fact our largest sample of the pinwheel tiling (≈ 22000 sites) had a lower z . The ratio between the whole bonds and sites gave $z \approx 5.5..$ which probably is due to a larger bond deficiency at the borders of the sample. For comparison, this pairs of values for the other lattices coincided up to a less than a percent.

We restrict our study to determining of the redundant bonds density in these lattices (for different bond dilutions). As it will be shown further this is sufficient for estimation of the rigidity percolation threshold.

In general, a d -dimensional lattice with n sites and no bonds between them will have $d.n - d(d-1)/2$ (in the plane $2n - 3$) mechanical degrees of freedom (or in the language of rigidity: floppy modes, or zero frequency modes). If now bonds are put between sites the number of floppy modes will decrease. If we neglect the angular forces, as it is accepted in the central-force percolation model, each bond will decrease the floppy modes at most by one. (Exactly said: by one or zero.) If no change occur in the number of floppy modes we speak about over-constraining or redundant bond.

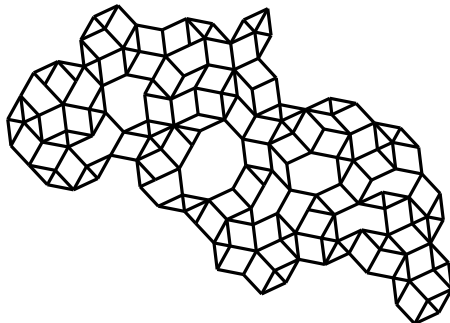


Figure 2: A part of rigid cluster (without the redundant bonds) in the “ferro” variant of the Penrose tiling ($p = 0.83$).

Now, the task is one to differ, in a network of rigid bars and joints, which bonds are redundant. In fact unambiguous decision for a certain bond could not exist for an already built construction. As was mentioned previously, in a square with diagonals one of the diagonals is redundant. In fact, each of the 6 bonds in this construction could be thought as the redundant one.

In the count of floppy modes the case of redundant bonds should be acknowledged so $F = 2n - (m - R)$, where F is the total number of floppy modes for the given (twodimensional) lattice, m is the number of added bonds and R are the redundant amongst them. Since the number of all bonds for a non-diluted (infinite) lattice is $zn/2$ (where z is the mean coordination number), the number of floppy modes per degree of freedom¹ ($f = F/2n$) can be written as:

$$f = 1 - p \frac{zn}{2} \frac{1}{2n} - \frac{R}{2n}$$

where p is the proportion of present bonds, or:

$$f = 1 - p \frac{z}{4} - r \tag{1}$$

where r is the number of redundant bonds per degree of freedom. If one neglects r , a mean-field-like (or Maxwell [2]) prediction, for the rigidity percolation threshold, could be done: $p_c^* = 4/z$.

The number of floppy modes(F) is (roughly) proportional to the number of rigid clusters for the system (if the isolated sites are counted as well). Roughly, because a site may belong to more than one rigid cluster. In analogy with the ordinary percolation model[17] one can argue [6] that f should behave as a free energy density, so its second derivative will follow power law near to the (real) percolation threshold:

¹of the unconstrained lattice

	\bar{z}	p_c	$4/z$
periodic triangular	6	$0.661 \pm 0.002^\dagger$	$2/3$
pinwheel	$6(5.5..)^\ddagger$	0.69 ± 0.01	$2/3(0.727..)^\ddagger$
Penrose ("ferro")	4.764...	0.836 ± 0.002	0.8396..
Octagonal(f)	5.17..	0.769 ± 0.002	0.774..
Dodecagonal(f)	4.27...	0.938 ± 0.001	0.937..

† a better result is given in [6]: 0.6602 ± 0.0003 ;

‡ the second numbers are the actual values for the largest studied sample (150×150)

(The size of the other lattices was up to 500×500)

Table 1: Rigidity percolation thresholds (bond dilution) for aperiodic lattices. (The triangular lattice is studied to test the estimation method.)

$$f'' \propto |p - p_c|^{-\alpha}$$

where α is a "specific-heat like" exponent. Integrating twice we can obtain the following form for f :

$$f(p) = b_1 + b_2 p + b_3 |p - p_c|^{2-\alpha} \quad (2)$$

Now comparing 2 and 1 we can use the data obtained for r to estimate p_c and (eventually) α (see Eq. 3 below).

In order to determine the rigidity percolation thresholds and the exponent α for the four aperiodic lattices the following procedure was established. The sites of a lattice are labeled with consecutive numbers and all their bonds are identified by the 2 numbers labeling the sites at their ends. The pairs of integers representing bonds are input with some probability p into a program which determines the number of dependent bonds in the formed subset. Any such subset describes in fact a particular configuration. The collected data consists in the number of dependent bonds monitored as a function of the varying probability p . We assume that they can be approximated satisfactorily (see above) by a function of the type

$$r(p) = a_1 + a_2 p + a_3 |p - a_4|^{a_5} \quad (3)$$

where a_1, a_2, a_3 being arbitrary parameters of no interest. While a_4 and a_5 should give estimations for the percolation threshold (p_c) and the "specific-heat-like" critical exponent (α) $a_4 \rightarrow p_c$ and $a_5 \rightarrow 2 - \alpha$.

The size of the lattices studied was of size up to $\approx 500 \times 500$ tile edge lengths. The pinwheel tiling was smaller: 150×150 . It was generated by iterative applying[18] the generating substitution rule[15]. The other three lattice were obtained by a recursive implementation[19] of the de Bruijns' N-grid method[20].

We counted the redundant bonds for lattices with different size and different bond dilutions, $q = 1 - p$ where p is the probability for present bond. We usually

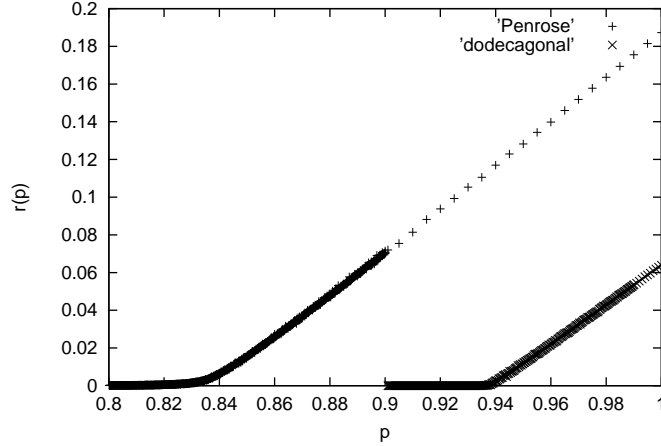


Figure 3: The redundant bonds per degree of freedom $r(p)$ for the “ferro” variants of the Penrose lattice (left curve) and the dodecagonal lattice. Each data point represents the result for *one* sample. The full lattices have $\approx 300\,000$ sites each.

run *one sample* for each p value, but we used about 1000 different values of p for each size. Usual practice was to use different pseudo random number sequence for each run.

Using a Marquard - Levenberg based optimization routine the parameters of a best fit with Eq.3 were estimated. This treatment of data appeared robust regarding the parameter a_4 (the percolation threshold). In opposite the other parameters appeared highly correlated and were depending on system size and the interval of values for p within the “measurements” were made. The larger interval (say, $p \in [0.6 - 0.9]$ for the Penrose tiling) led to smaller values for a_5 (approaching 1 as one could expect from the figure). One should suppose that using an interval closer to the threshold would give a better estimate, but this time the finite size effects start to influence. We attempted finite-size scaling but (probably due to the linear term in Eq.3) we could not extract consistent data. It seems that just counting the total number of redundant bonds is not sufficient to estimate the exponent α .

As we already mentioned the estimates for p_c were surprisingly stable regarding the changes of systems size and the interval for p used in the fit. Of course some deviations were seen and we have to made extrapolation to infinite size and to choose the interval for varying of p . We used mostly the results for interval of p within 6-7% above and 2-3% below the rough estimate for p_c .

The obtained results are summarized in Table 1. For a triangular lattice the percolation threshold has been already established with great accuracy [6] to be

0.6602 ± 0.0003 while the Maxwell prediction is $2/3$. The procedure utilized here gives 0.661 ± 0.002 which supports our results for the other lattices.

We check these results by adding a kind of bus-bars to two opposite edges of the lattice sample[9]. We simply used $p = 1$ when entering into the pebble game program the bonds within the left and right edge of the “sample”. After reading all bonds we added *one more* bond to connect a site from the left edge to a site to the right one. If a spanning rigid cluster has already existed between these edges, the new (long-range) bond should be redundant. We studied in this way the largest lattice sizes by fixing three values for p : $p = p_c - \Delta p_c$; $p = p_c$; $p = p_c + \Delta p_c$; where Δp_c was equal to the estimated “error bars” given in the Table 1. We made typically 100 runs for each value of p . It appeared that we have chosen the proper interval for p to estimate p_c in our fits of $r(p)$.

When compare the entries in the last two columns of the table one can see that the mean-field like approximation works very well and it becomes better when the percolation threshold is closer to 1. When look on the curves on Fig.3 one can mention (in fact H.J. Hermann was who mentioned) that almost 90% of the bonds added above the percolation threshold are redundant. So, the building parts of the spanning rigid cluster exist even below the threshold and only few bonds are needed to connect them in the rigid structure which spans the sample.

In conclusion one may summarize the results of this work as follows: it was studied for the first time the rigidity percolation model for some aperiodic lattices. Four typical representatives of these lattices were studied: the Penrose tiling from two rhombuses, the Ammanns’ octagonal tiling, the Socolars’ dodecagonal tiling, and the “pinwheel” tiling constructed by J. Conway. It was shown that the counting of redundant bonds in rigidity percolation models on these tilings is sufficient to locate the percolation threshold with a good precision. The rigidity percolation “generic” thresholds for bond dilution were estimated and compared with the Maxwell approximation. The results show that the critical region is very narrow for this lattices as is the case for triangular lattice, so the Maxwell approximation (to neglect the redundant bonds) gives very good estimates for the percolation thresholds.

It would be interesting, the obtained here “generic” thresholds to be compared with results from force equilibrium calculations on “perfect” aperiodic lattices. One could expect that the difference should be smaller than for triangular lattices, since so c. diode effect in aperiodic lattices is less pronounced.

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